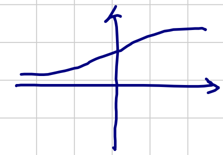
Stanford Machine Learning — Support Vector Machine

1. Large Margin Classification.

Optimization objective.



· logistic regression $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$.

- if $y=1$, we want $h_\theta(x) \approx 1 \Rightarrow \theta^T x \gg 0$

  $y=0$, $h_\theta(x) \approx 0 \Rightarrow \theta^T x \ll 0$.

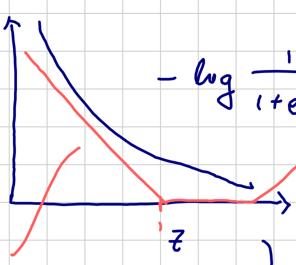
· cost of example: $-[y \log h_\theta(x) + (1-y) \log(1-h_\theta(x))]$

$$= \underbrace{-y \log \frac{1}{1+e^{-\theta^T x}}}_{①} \underbrace{- (1-y) \log\left(1 - \frac{1}{1+e^{-\theta^T x}}\right)}_{②}$$

①

If $y=1$ (want $\theta^T x \gg 0$)

$z = \theta^T x$.



$-\log \frac{1}{1+e^{-z}}$

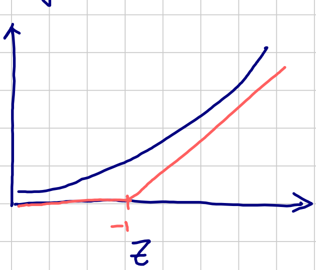
flat portion $cost_1 z$

support vector machine.

straight line portion

large z, small cost contribution.

② If $y=0$, we want ($z = \theta^T x \ll 0$)



$-\log\left(1 - \frac{1}{1+e^{-z}}\right)$ $cost_0 z$

Support Vector Machine

· Logistic Regression.

$$\min_\theta \frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)} \underbrace{\left(-\log h_\theta(x^{(i)})\right)}_{cost_1(\theta^T x^{(i)})} + (1-y^{(i)})\cdot \underbrace{\left(-\log(1-h_\theta(x^{(i)}))\right)}_{cost_0(\theta^T x^{(i)})}\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

· Support Vector Machine.

$$\min_\theta \frac{1}{m}\cdot \sum_{i=1}^{m} y^{(i)}\cdot cost_1(\theta^T x^{(i)}) + (1-y^{(i)})\cdot cost_0(\theta^T x^{(i)}) + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

· convention : (1) remove $(\frac{1}{m})$ term → does not change θ min

(2) log. reg format $A + \lambda B$.

S.V.M format $cA + B$ (diff. way of parametrization of tradeoffs)

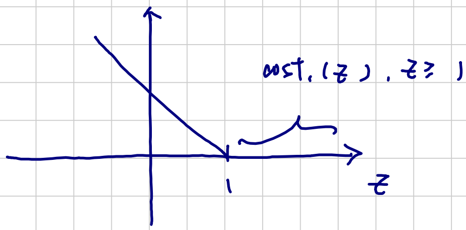
⇒ Support Vector Machine

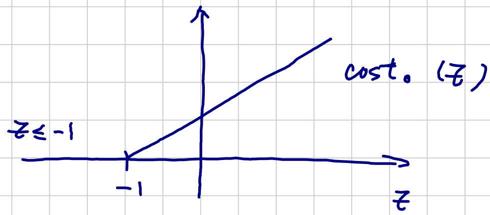
$$\boxed{\min_\theta C\sum_{i=1}^{m}\left[y^{(i)}\cdot cost_1(\theta^T x^{(i)}) + (1-y^{(i)})\cdot cost_0(\theta^T x^{(i)})\right] + \frac{1}{2}\sum_{j=1}^{n}\theta_j^2}$$

· Hypothesis $h_\theta(x) = \begin{cases} 1, & \text{if } \theta^T x \geq 0 \\ 0, & \text{otherwise} \end{cases}$ form of hypothesis.

Large Margin Intuition

- Recall :





- If $y=1$, we want $\theta^T \cdot x \geq 1$ (not just ≥ 0)

  $y=0$, we want $\theta^T \cdot x \leq -1$ (not just < 0)

  ↓

  for logistic regression

- Here, we shift the threshold to be more conservative.

- SVM Decision Boundary.

  (1) setting $C = 10{,}000$.

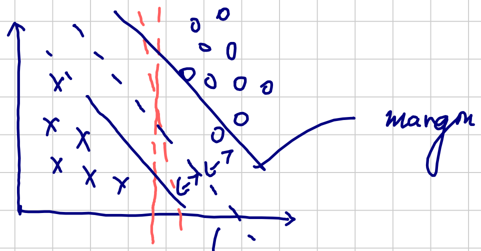
$$\min_\theta \; C \sum_{i=1}^{m} \left[y^{(i)} cost_1(\theta^T x^{(i)}) + (1-y^{(i)}) cost_0(\theta^T \cdot x^{(i)}) \right] + \frac{1}{2}\sum_{j=1}^{n} \theta_j^2$$

Whenever $y^{(i)} = 1$, we need $\theta^T x^{(i)} \geq 1$

$y^{(i)} = 0$, $\theta^T x^{(i)} \leq -1$

$$\Rightarrow \min. \; \cancel{C} \cdot 0 + \frac{1}{2}\sum_{j=1}^{n} \theta_j^2 \quad \text{s.t.} \quad \begin{matrix} \theta^T x^{(i)} \geq 1 & \text{if } y^{(i)} = 1 \\ \theta^T \cdot x^{(i)} \leq -1 & \text{if } y^{(i)} = 0 \end{matrix}$$

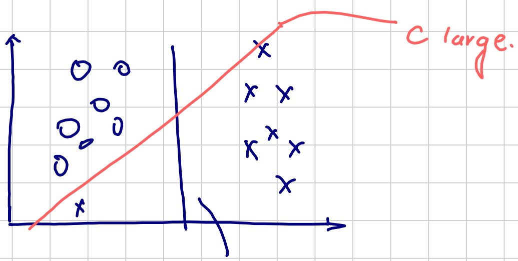
SVM Decision Boundary: Linearly Separable Case.



SVM = Large Margin classifier.

larger min. distance to data points. (large margin)

Large Margin classifier in Presence of Outliers



C not too large , C similar to $\frac{1}{\lambda}$

if λ small, then we have overfitting due to outliers.

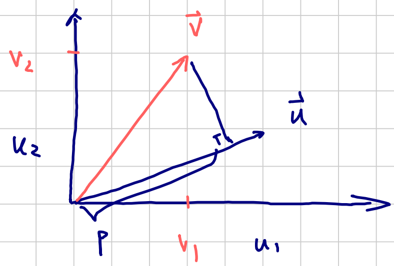
Mathematics Behind Large Margin Classification

1 Review.

(1) Vector inner product.

$$\vec{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \quad \vec{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

inner product $= u^T \cdot v$.



$\|\vec{u}\|$ = length of $\vec{u}$ $= \sqrt{u_1^2 + u_2^2} \in \mathbb{R}$.

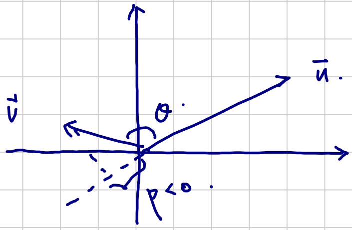
p = length of $\text{projection}_{\vec{u}}\, \vec{v}$. (signed).

$u^T v = p \cdot \|\vec{u}\|$. (Can be shown)

so. $\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}^T \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = p \cdot \|\vec{u}\| \quad \in \mathbb{R}^2$

$\Rightarrow \boxed{u_1 v_1 + u_2 v_2 = p \cdot \|\vec{u}\|}$ Theorem.

· Sign of p.



$p<0$ if $\theta > 90°$.

2. SVM Decision Boundary

$$\boxed{\min_\theta \frac{1}{2}\sum_{j=1}^{n}\theta_j^2}$$

s.t. $\theta^T \cdot x^{(i)} \geq 1$ if $y^{(i)} = 1$

$\theta^T \cdot x^{(i)} \leq -1$ $y^{(i)} = 0$

simplification $\theta_0 = 0$, $n = 2$ $\Rightarrow$ $\min_\theta \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 = \frac{1}{2}(\theta_1^2 + \theta_2^2)$

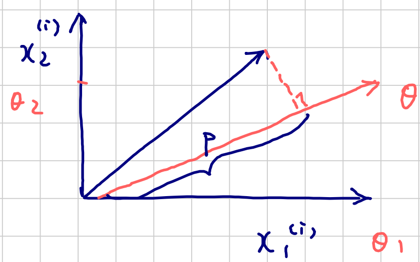
$= \frac{1}{2}\left(\sqrt{\theta_1^2 + \theta_2^2}\right)^2$

$= \frac{1}{2}\|\theta\|^2$, where $\theta = \begin{pmatrix}\theta_1 \\ \theta_2\end{pmatrix}$

$\theta^T x^{(i)} = ?$

$\downarrow \quad \downarrow$

$u^T \quad v$



$\theta^T x^{(i)} = p^{(i)} \cdot \|\theta\|$

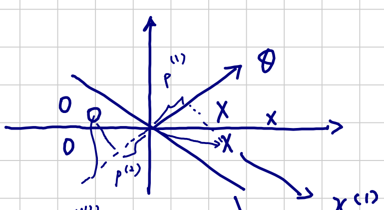
$= \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)}$

$\Rightarrow \min_\theta \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 = \frac{1}{2}\|\theta\|^2$ s.t. $p^{(i)} \cdot \|\theta\| \geq 1$, if $y^{(i)} = 1$

$p^{(i)} \cdot \|\theta\| \leq -1$, if $y^{(i)} = 1$

where $p^{(i)} = \text{proj}_\theta x^{(i)}$

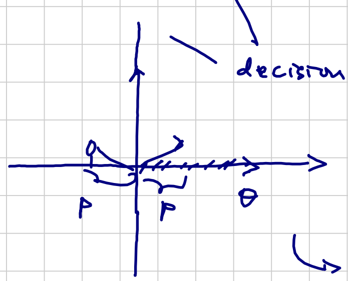
simplification.



$p^{(i)}$ small, but $p^{(i)} \cdot \|\theta\| \geq 1$

$\Rightarrow$ need large θ $\longleftrightarrow$ min. $\frac{1}{2}\|\theta\|^2$

conflict.



decision boundary

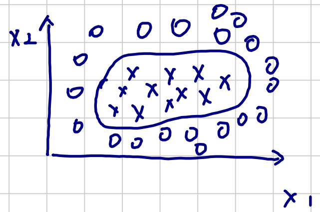
Now $p^{(i)}$ bigger, we can have a smaller θ $\Rightarrow$ $\min_\theta \frac{1}{2}\|\theta\|^2$ ✓

$\hookrightarrow$ SVM choose this decision boundary

Simplification. $\theta_0 = 0$ $\Rightarrow$ decision passes through boundary.

2. Kernels.

· Non-linear decision boundary



$$h_\theta(x) = \begin{cases} 1, & \text{if } \theta_0 + \theta_1 x_1 + \cdots \geq 0. \\ 0, & \text{otherwise}. \end{cases}$$

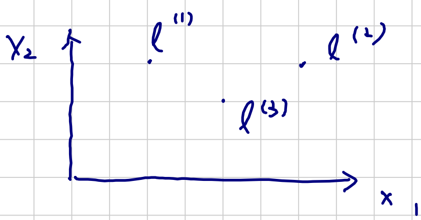
$\Rightarrow$ Can be written as $\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 + \cdots$

$f_1 = x_1$, $f_2 = x_2$, $f_3 = x_1 x_2$, $f_4 = x_1^2$, $f_5 = x_2^2 \cdots$

↳ Is there a better choice of features

$f_1, f_2, \ldots$? (high order polynomials are expensive)

· Kernel.



Given x, compute new feature depending on proximity to landmarks $\ell^{(1)}$, $\ell^{(2)}$, $\ell^{(3)}$.

$f_1 = \text{similarity}(x, \ell^{(1)})$

square of euclidean distance.

$$= \exp\left(- \frac{\|x - \ell^{(1)}\|^2}{2\sigma^2}\right)$$

$\vdots$

Kernel. $\leftarrow$ $f_i = \text{similarity}(x, \ell^{(i)})$

$k(x, \ell^{(i)})$

$$= \exp\left(- \frac{\|x - \ell^{(i)}\|^2}{2\sigma^2}\right)$$

↳ A specific type of kernel (gaussian).

· Kernels and similarity.

· note: $\|x - \ell^{(i)}\|^2$ can be written as $\sum_{j=1}^{n} (x_j - \ell_j^{(i)})^2$

(1) If $x \approx \ell^{(1)}$, then $\|x - \ell^{(1)}\|^2 \approx 0$.

$\Rightarrow$ $\boxed{f_1 \approx \exp\left(- \frac{0}{2\sigma^2}\right) = 1}$

(2) If x far. $\ell^{(1)}$, then $\|x - \ell^{(1)}\|^2$ large

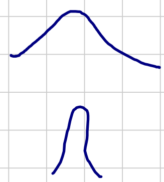
$\boxed{f_1 \approx 0}$

- Each landmark defines a new feature. $\ell^{(i)} \Leftrightarrow f_i$

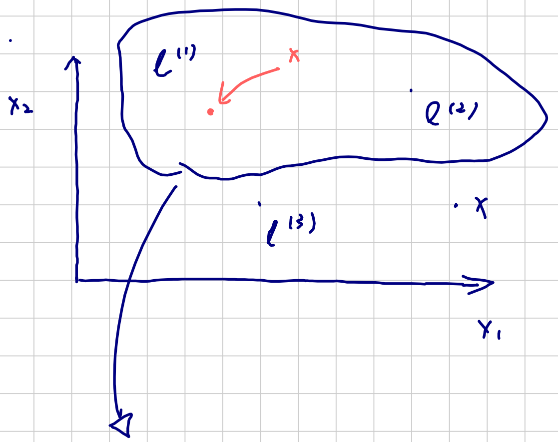
Ex.

- $\ell^{(1)} = \begin{pmatrix} 3 \\ 5 \end{pmatrix}$ $\quad f_1 = \exp\left(- \frac{\| x - \ell^{(1)} \|^2}{2\sigma^2} \right)$, $\sigma^2 = 1$. (variance).

- as σ^2 incr, f falls slower.
  decr. faster



Ex.



learned decision boundary.

Predict "1" when

$$\boxed{\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 \geq 0} \quad (*)$$

① $f_1, f_2, f_3 \longrightarrow x$.

$\theta_0 = -0.5$, $\theta_1 = 1$, $\theta_2 = 1$, $\theta_3 = 0$.

$(*) \Rightarrow f_1 \approx 1$ (x close to $\ell^{(1)}$)

$f_2 \approx 0$, $f_3 \approx 0$

$\Rightarrow \theta_0 + \theta_1 \cdot 1 + \theta_2 \cdot 0 + \theta_3 \cdot 0 = -0.5 + 1$

$= 0.5 \geq 0 \Rightarrow$ predict. "1"

$(*) \Rightarrow f_1, f_2, f_3 = 0$

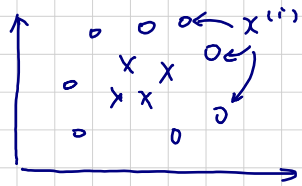
$\theta_0 + \cdots = -0.5 < 0 \Rightarrow$ predict "0"

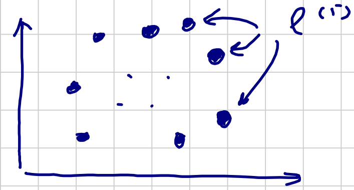
$\Rightarrow$ for points close to $\ell^{(1)}, \ell^{(2)} \to$ predict 1.

far. 0

· Choosing landmark.

- where do we get $\ell^{(1)}, \ell^{(2)}, \ell^{(3)}$?





predict $y=1$ if $\sum_0 \theta_i f_i \geq 0$.

- features are measuring on how close to training examples, given a x.

- Given. $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), (x^{(3)}, y^{(3)}) \dots (x^{(m)}, y^{(m)})$

$\Rightarrow$ choose $\ell^{(1)} = x^{(1)}, \ell^{(2)} = x^{(2)}, \dots, \ell^{(m)} = x^{(m)}$.

- given example x,

$$f_1 = \text{similarity}(x, \ell^{(1)}) \quad \ell^{(1)} \to x^{(1)}$$
$$f_2 = \text{similarity}(x, \ell^{(2)}) \quad \ell^{(2)} \to x^{(2)}$$
$$\vdots$$

$$\Rightarrow f = \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_m \end{bmatrix} \qquad f_0 = 1.$$

→ each element rep. how close the vector x is to each landmark. $\ell^{(i)}$.

· For training example $(x^{(i)}, y^{(i)})$

$$x^{(i)} \longrightarrow \begin{array}{l} f_1^{(i)} = \text{sim}(x^{(i)}, \ell^{(1)}) \\ f_2^{(i)} = \text{sim}(x^{(i)}, \ell^{(2)}) \\ \vdots \\ f_m^{(i)} = \text{sim}(x^{(i)}, \ell^{(m)}) \end{array} \longleftarrow f_i^{(i)} = \text{sim}(x^{(i)}, \ell^{(i)}) = \text{sim}(x^{(i)}, x^{(i)}) = 1.$$

$\ell^{(i)} \to x^{(i)}$

$$x^{(i)} \in \mathbb{R}^{n+1} \quad (0,\dots,n) \quad \Rightarrow \quad f^{(i)} = \begin{pmatrix} f_0^{(i)} \\ f_1^{(i)} \\ \vdots \\ f_m^{(i)} \end{pmatrix} \qquad \boxed{f_0^{(i)} = 1}$$

SVM with Kernels

① Hypothesis : given x, compute features $f \in \mathbb{R}^{m+1}$

predict "$y=1$" if $\theta^T f \geq 0 \Rightarrow \sum_{0}^{m} \theta_i f_i \geq 0$

② Training :

$$\min_{\theta} C \sum_{i=1}^{m} y^{(i)} \cdot cost_1(\theta^T \cdot f^{(i)}) + (1-y^{(i)}) \cdot cost_0(\theta^T \cdot f^{(i)}) + \frac{1}{2} \sum_{j=1}^{m} \theta_j^2$$

$n = m$!

③ Implementation note.

· $\sum_{j=1}^{m} \theta_j^2 = \theta^T \cdot \theta$, $\theta = \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_m \end{pmatrix}$ ignoring θ_0.

· often, one can also scale the θ. i.e. $\theta^T \cdot \underline{M} \theta$.

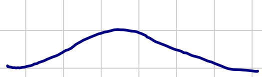
· $M \rightarrow \uparrow$ computation efficiency.

SVM Parameters

$C \left(= \frac{1}{\lambda}\right)$
- large C : low bias, high variance (small λ)
- small C : high bias, low variance. (large λ)

σ^2 Large σ^2 : features f_i vary more smoothly.

High bias, lower variance (changes too slow)



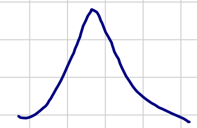
Guassian kernel

$$\exp\left(- \frac{\|x - l^{(i)}\|^2}{2\sigma^2} \right)$$

small σ^2 . features f_i vary less smoothly.

lower bias, high variance

(changes abruptly) .



3. SVM in Practise. : Using a SVM.

- Use SVM software package (eg. liblinear, libsvm) to solve for SVM.

- Specification

  (1) Choice of parameter C.

  (2) choice of kernal. (similarity function)

a. No kernel. ("linear kernel")

. Predict $y=1$ if $\theta^T x > 0$

↳ good for large n (# of features) $x \in \mathbb{R}^{n+1}$.

small m. (small data set)

b. Guassian Kernel.

① $f_i = \exp\left(-\frac{\|x - l^{(i)}\|^2}{2\sigma^2}\right)$, where $l^{(i)} = x^{(i)}$.

Need to choose σ^2

↳ good for small n. ($x \in \mathbb{R}^{n+1}$)

and/or large m.

② Kernel (similarity function)

function $f = \text{kernel}(x1, x2)$

$$f = \exp\left(-\frac{\|x1 - x2\|^2}{2\sigma^2}\right)$$

return .

* Note: perform feature scaling before using the Guassian kernel.

C. Other choices of kernel.

· not all similarity functions similarity (x, l) make valid kernels.

[Need to classify technical condition called "Mercer's theorem" to make sure SVM packages' optimizations run correctly and not diverge]

· Available options.

(1) polynomial kernel $k(x, l) = (x^T l)^2$,

$(x^T l)^3$, $(x^T l + 1)^3$.

$(x^T l + 5)^4$

two parameters c, d

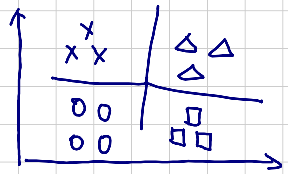
s.t. $\boxed{(x^T l + c)^d}$.

text.

(2) Esoteric: string kernels, chi-square kernel,

histogram kernel, ...

· Multiclass classification.



$y \in \{1, 2, 3 \dots k\}$.

· Pick class i with largest

$(\theta^{(i)})^T x$.

· Logistic Regression vs. SVMs.

n: # features. m = # examples

(1) $n >> m$. e.g. $n = 10000$, $m = 10 \dots 1000$.

- logistic regression
- SVM w/o kernel. (linear kernel)
- not enough data.

(2) n small, m intermediate $n = 1 \dots 1000$.
$m = 10, \dots 10{,}000$

- SVM with Guassian Kernel.

(3) n small, m large. $n = 1\text{-}1000$, $m = 50{,}000+ \dots$

- Create / add more features

↓

Use
- logistic regression
- SVM without a kernel.

→ similar algorithm (similar output, slight difference in efficiency)

- Neural network: likely to work with any, may be slower to train.